Elastic energy for reflection-symmetric topologies

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Abstract

Nematic liquid crystals in a polyhedral domain, a prototype for bistable displays, may be described by a unit-vector field subject to tangent boundary conditions. Here we consider the case of a rectangular prism. For configurations with reflection-symmetric topologies, we derive a new lower bound for the one-constant elastic energy. For certain topologies, called conformal and anticonformal, the lower bound agrees with a previous result. For the remaining topologies, called nonconformal, the new bound is an improvement. For nonconformal topologies we derive an upper bound, which differs from the lower bound by a factor depending only on the aspect ratios of the prism.

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1 Introduction

Present-day liquid crystal displays (eg twisted nematic) are based on *monostable* cells, wherein, in the absence of external fields, the orientations of the liquid crystal molecules assume a single (spatially varying) mean configuration which is effectively transparent to incident polarised light. To produce and maintain optical contrast, voltage pulses, which reorient the molecules, must be continually applied. There is considerable interest in developing *bistable* cells, which support two (and possibly more) stable liquid crystal configurations with contrasting optical properties. In bistable cells, power is needed only to switch between the two states. One mechanism for engendering bistability is the cell geometry [1, 2, 3]; nematic liquid crystals in prototype cells with polyhedral geometrical features (eg, ridges, or posts) are found to support multiple configurations.

As a simple model for such systems, we consider the mean local orientation of a nematic liquid crystal in a polyhedral domain as described by a director field $\mathbf{n}$ subject to suitable boundary conditions. The situation we consider, strong azimuthal anchoring, is described by *tangent boundary conditions*. Tangent boundary conditions require that, on a face of the domain, $\mathbf{n}$ lies tangent to the face, but is otherwise unconstrained. This implies that on the edges of the polyhedron, $\mathbf{n}$ is parallel to the edges, and therefore is necessarily discontinuous at the vertices. We restrict our attention to director fields which are continuous away from the vertices (ie, as continuous as possible). In this case we can unambiguously assign an orientation to the director (as the domain is simply connected), and regard $\mathbf{n}$ as a unit-vector field.

In [4], we give a complete topological classification of continuous tangent unit-vector fields in a convex polyhedron. An extension to the nonconvex and periodic cases, along with a general procedure for analysing a large class of such classification problems, is given in [5]. In [6] we obtain a lower bound for the one-constant energy in terms of certain topological invariants, the trapped areas. The case of a rectangular prism is considered in [7], where we also derive an upper bound for the equilibrium (infimum) energy for a large family of topologies called reflection-symmetric conformal and anticonformal. For these topologies, the ratio of the upper and lower bounds depends only on the aspect ratios of the prism. We also show that topologically nontrivial behaviour of configurations close to equilibrium may concentrate near the edges, or may be smoothly distributed, depending on the aspect ratios.

In this paper we consider again the case of a rectangular prism, and improve and extend the previous results of [7]. Specifically, we derive a new lower bound for the energy of reflection-symmetric topologies, expressed in

terms of different invariants, namely the wrapping numbers. In general, the new lower bound is an improvement on the previous one. We also extend the analysis to all reflection-symmetric topologies, not just conformal and anticonformal ones.

While liquid crystal applications are a principal motivation for this work, the problems are also of intrinsic mathematical interest. Minimizers of the one-constant energy may be regarded as harmonic maps from a Euclidean polyhedron to the two-sphere S^2. The study of harmonic maps between Riemannian manifolds is an extensive field, and connections to problems in liquid crystals are well known [8]. For manifolds with boundary, the regularity of minimisers for the Dirichlet problem for harmonic maps with sufficiently smooth (C^2) boundary and Dirichlet data are investigated in [9]. However, less appears to be known about the case of manifolds with Lipschitz boundary, eg domains with corners, and for natural, eg tangent boundary conditions. There are recent strong results on the existence, uniqueness and regularity of minimisers for the Dirichlet problem for harmonic maps of fixed homotopy type between Riemannian polyhedra for target spaces of negative curvature [10]. However, it appears to be much more difficult to obtain corresponding results for target spaces of positive curvature, eg S^2, which we encounter in liquid crystals problems.

The paper is organised as follows. The topological classification of tangent unit-vector fields in a rectangular prism is reviewed in Section 2. We introduce the reflection-symmetric topologies, which are characterised by certain invariants – the edge signs e, kink numbers k and trapped area Ω – associated with one of the prism vertices. In Section 3 we derive a lower bound for the one-constant elastic energy. This turns out to depend on the absolute values of the wrapping numbers (which may be expressed in terms of e, k and Ω). For certain topologies, called conformal and anticonformal, for which the wrapping numbers all have the same sign, the lower bound can be expressed in terms of the trapped area alone, and coincides with the result previously derived in [6, 7]. Conformal and anticonformal topologies are characterised in Section 4, where it is shown that these are precisely the topologies which have conformal and anticonformal representatives of the type considered in [7]. In Section 5 we introduce representative configurations for nonconformal topologies, and derive from them an upper bound for the elastic energy. This differs from the lower bound of Section 2 by a factor depending only on the aspect ratios. Appendix A contains a derivation of a formula for the kink numbers of conformal and anticonformal configurations.

2 Reflection-symmetric topologies

Let us briefly recall the results concerning the classification of continuous tangent unit-vector fields $\mathbf{n}$ on a rectangular prism P. For convenience, we let P denote the prism without its vertices, so that $\mathbf{n}$ is continuous on P. For definiteness, we take the prism to be given by $0 \le r_j \le L_j$, with edge lengths L_j ordered so that $L_x \ge L_y \ge L_z$. At each vertex of P, denoted $\mathbf{v} = (v_x, v_y, v_z)$, we associate to $\mathbf{n}$ a set of topological invariants, namely the *edge signs*, *kink numbers* and *trapped area*. The edge signs, denoted $e_j^{\mathbf{v}}$, determine the signs of $\mathbf{n}$ on the edges at $\mathbf{v}$ relative to the coordinate unit vectors, ie

$$\mathbf{n}(x, v_y, v_z) = e_x^{\mathbf{v}}\,\hat{\mathbf{x}}, \quad 0 \le x \le L_x, \tag{1}$$

and similarly for $e_y^{\mathbf{v}}$ and $e_z^{\mathbf{w}}$. (Of course, this designation is redundant; the edge signs $e_j^{\mathbf{v}}$ and $e_j^{\mathbf{w}}$ at vertices $\mathbf{v}$ and $\mathbf{w}$ joined by an edge parallel to the j-axis are necessarily the same.)

The integer-valued kink numbers, denoted $k_j^{\mathbf{v}}$, count the windings of $\mathbf{n}$ along a path about $\mathbf{v}$ on the face normal to $\hat{\boldsymbol{\jmath}}$. By convention, the paths are taken to be positively oriented with respect to the outward normal through the centre of the face. The minimum possible winding (a net rotation of $\pm\pi/2$) is assigned a kink number of zero. Nonzero windings are designated positive or negative according to their orientation with respect to the outward normal (either $\hat{\boldsymbol{\jmath}}$ or $-\hat{\boldsymbol{\jmath}}$). The continuity of $\mathbf{n}$ (in particular, the absence of singularities on the surface of P) implies that the kink numbers on each face satisfy a sum rule [4]; for example, on one of the faces F normal to $\hat{\mathbf{z}}$, it turns out that

$$\sum_{\mathbf{v}\in F} \left(k_z^{\mathbf{v}} - \tfrac{1}{4}(-1)^{v_x/L_x}(-1)^{v_y/L_y} e_x^{\mathbf{v}} e_y^{\mathbf{v}}\right) = 0. \tag{2}$$

Analogous rules hold for the other faces.

The last invariant, the trapped area, denoted $\Omega^{\mathbf{v}}$, is the oriented area on the unit two-sphere S^2 of the image, $\mathbf{n}(C^{\mathbf{v}})$, of a surface, $C^{\mathbf{v}}$, which separates $\mathbf{v}$ from the other vertices. That is, letting (θ, ϕ) denote polar coordinates on S^2,

$$\Omega^{\mathbf{v}} = \int_{\mathbf{n}(C^{\mathbf{v}})} \sin\theta \, d\theta \wedge d\phi. \tag{3}$$

Expressed as an integral over $C^{\mathbf{v}}$ itself, $\Omega^{\mathbf{v}}$ is given by

$$\Omega^{\mathbf{v}} = \int_{C^{\mathbf{v}}} \mathbf{D} \cdot \hat{\mathbf{C}}^{\mathbf{v}} \, dS. \tag{4}$$

Here $\hat{\mathbf{C}}^{\mathbf{v}}$ is the outward-oriented unit normal on $C^{\mathbf{v}}$ ($\hat{\mathbf{C}}^{\mathbf{v}}$ points towards $\mathbf{v}$)

and dS is the area element, while the vector field $\mathbf{D}(\mathbf{r})$ is given by

$$D_j = \tfrac{1}{2}\epsilon_{jkl}(\partial_k \mathbf{n} \times \partial_l \mathbf{n}) \cdot \mathbf{n}. \tag{5}$$

That (3) and (5) are equivalent follows from the fact that

$$\mathbf{D} \cdot \hat{\mathbf{C}}^{\mathbf{v}} = \det d\mathbf{n}_{C^{\mathbf{v}}}, \tag{6}$$

where $d\mathbf{n}_{C^{\mathbf{v}}}$ denotes the Jacobian of the restricted map $\mathbf{n}_{C^{\mathbf{v}}} : C^{\mathbf{v}} \to S^2$ (and, as above, $C^{\mathbf{v}}$ is oriented with respect to the outward normal).

For a rectangular prism, the trapped areas are necessarily odd multiples of $\pi/2$ (the area of a right spherical triangle), and for given values of the edge signs and kink numbers, the allowed values of the trapped areas differ by multiples of 4π (whole coverings of the sphere) – see (13) below. The continuity of $\mathbf{n}$ (the absence of singularities inside P) implies the sum rule

$$\sum_{\mathbf{v}} \Omega^{\mathbf{v}} = 0. \tag{7}$$

One can show ([4]) that the edge signs, kink numbers and trapped areas are indeed topological invariants (ie, they are invariant under continuous deformations of $\mathbf{n}$ that preserve the tangent boundary conditions) and that two tangent unit-vector fields on P are homotopic if and only if their invariants are the same. For convenience we have slightly adapted the notation of [4] to suit the case of prisms (the conventions, however, are the same).

In what follows we restrict our attention to a subset of the allowed prism topologies which we call *reflection symmetric*. Let $\mathbf{v}$ and $\mathbf{w}$ denote a pair of vertices related by a reflection though a midplane of the prism (and therefore joined by an edge). For reflection-symmetric topologies, the edge signs at $\mathbf{v}$ and $\mathbf{w}$ are the same while the kink numbers and trapped areas differ by a sign. That is,

$$e_j^{\mathbf{v}} = e_j^{\mathbf{w}}, \quad k_j^{\mathbf{v}} = -k_j^{\mathbf{w}}, \quad \Omega^{\mathbf{v}} = -\Omega^{\mathbf{w}}. \tag{8}$$

It follows that at vertices related by two reflections (ie, at diagonally opposite corners of a face), the invariants are the same, while the invariants of vertices related by three reflections (at diagonally opposite corners of the prism) are related as in (8).

For reflection-symmetric topologies the invariants are determined by their values at a single vertex. For definiteness we take this vertex to be the origin, and henceforth denote the invariants simply as (e, k, Ω). The surface separating the origin from the other vertices will be denoted by C. It is straightforward to check that (8) implies that the sum rules (2) and (7) are automatically satisfied.

The terminology stems from the fact that every reflection-symmetric topology has a reflection-symmetric representative, ie a configuration $\mathbf{n}$ which is symmetric under reflections through the mid planes,

$$\mathbf{n}(x, y, z) = \mathbf{n}(L_x - x, y, z) = \mathbf{n}(x, L_y - y, z) = \mathbf{n}(x, y, L_z - z). \tag{9}$$

Let

$$R = \{\mathbf{r} \,|\, 0 \leq r_j \leq \tfrac{1}{2} L_j\} \tag{10}$$

denote the octant of the prism with the origin as vertex. Then a reflection-symmetric configuration is determined by its values in R. It is straightforward to verify that (9) implies the relations (8). Conversely, given a configuration $\mathbf{n}'$ with reflection-symmetric topology (e, k, Ω) but which is not itself reflection symmetric, we can construct a reflection-symmetric configuration $\mathbf{n}$ satisfying (9) with invariants (e, k, Ω) (just take $\mathbf{n} = \mathbf{n}'$ in the prism octant R and define $\mathbf{n}$ elsewhere via (9)).

In [4] we introduced certain additional integer-valued topological invariants, called *wrapping numbers*. As the preceding discussion implies, the wrapping numbers are not independent of the edge signs, kink numbers and trapped areas, but rather can be expressed in terms of them. We briefly recall the definition and properties of the wrapping numbers, as they are central to the discussion to follow.

Let $\mathbf{s}$ denote a regular value of $\mathbf{n}$ restricted to C. That is, on C, there is a finite number of points where $\mathbf{n}$ takes the value $\mathbf{s}$, and, at any such point, the Jacobian of the map $\mathbf{n}_C : C \to S^2$ is nonsingular, so that, from (6), $(\mathbf{D} \cdot \hat{\mathbf{C}})(\mathbf{s}) \neq 0$. The wrapping number at $\mathbf{s}$, denoted $w(\mathbf{s})$, is a signed count of the pre-images of $\mathbf{s}$ on C, denoted $\mathbf{r}_p$, the sign determined by whether $\mathbf{n}_C$ is orientation-preserving (+) or reversing (−) at $\mathbf{r}_p$. Thus

$$w(\mathbf{s}) = \sum_p \operatorname{sgn}\left[(\mathbf{D} \cdot \hat{\mathbf{C}})(\mathbf{r}_p)\right]. \tag{11}$$

To express the wrapping number in terms of the other invariants [4, 11], let $U_{p\epsilon}$ denote the disk of radius ϵ about $\mathbf{r}_p$ on C, and let $C - \sum_p U_{p\epsilon}$ denote C with these disks excised. Let ∂C denote the boundary of C and $\partial U_{p\epsilon}$ the boundary of $U_{p\epsilon}$. Choosing $\mathbf{s}$ as the south pole of the polar angles (θ, ϕ) in (3) and using Stokes' theorem, we get that

$$\Omega = \lim_{\epsilon \to 0} \int_{\mathbf{n}\left(C - \sum_p U_{p\epsilon}\right)} \sin\theta \, d\theta \wedge d\phi = \left(\int_{\mathbf{n}(\partial C)} - \lim_{\epsilon \to 0} \int_{\mathbf{n}\left(\sum_p \partial U_{p\epsilon}\right)} \right) (1 - \cos\theta) d\phi. \tag{12}$$

$\mathbf{n}(\sum_p \partial U_{p\epsilon})$ consists of p small circuits about $\mathbf{s}$, and the integral over these circuits in (12) gives, in the limit $\epsilon \to 0$, 4π times $w(\mathbf{s})$. $\mathbf{n}(\partial C)$ consists

of the spherical right triangle with vertices $e_j\hat{\boldsymbol{\jmath}}$, $j = x, y, z$, along with k_j circuits of the great circle normal to $\hat{\boldsymbol{\jmath}}$. Each great circle contributes $\pm 2\pi$ to the integral in (12) according to its orientation with respect to the polar axis through $\mathbf{s}$, while the spherical triangle contributes $\pm\pi/2$ (its signed area) or $\pm 7\pi/2$ according to whether or not it encloses $\mathbf{s}$. Keeping track of signs one gets

$$w(\mathbf{s}) = \tfrac{1}{4\pi}\Omega + \tfrac{1}{2}\sum_j \sigma_j k_j + e_x e_y e_z \times \begin{cases} -\frac{7}{8}, & \text{if } \sigma_j = \operatorname{sgn} e_j \text{ for all } j, \\ +\frac{1}{8}, & \text{otherwise.} \end{cases} \tag{13}$$

where $\sigma_j = \operatorname{sgn} s_j$. From (13) it is clear that $w(\mathbf{s})$ is a topological invariant. In fact, $w(\mathbf{s})$ can be defined so long as $\mathbf{s}$ does not lie in a coordinate plane (ie, even if $\mathbf{s}$ is not a regular value of $\mathbf{n}$) as the degree of a certain continuous $S^2 \to S^2$ map constructed by gluing $\mathbf{n} : C \to S^2$ to a reference map which coincides with $\mathbf{n}$ on the boundary ∂C [4].

(13) also implies that $w(\mathbf{s})$ depends only on the signs of the components of $\mathbf{s}$, ie on the octant of S^2 to which $\mathbf{s}$ belongs. In what follows, we label octants by a triple of signs $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, so that O_σ denotes the octant $\{\mathbf{s} \,|\, \operatorname{sgn} s_j = \sigma_j\}$. For convenience we let w_σ denote the value of $w(\mathbf{s})$ for $\mathbf{s} \in O_\sigma$. Summing over octants in (13), we get that

$$\Omega = \tfrac{1}{2}\pi \sum_\sigma w_\sigma \tag{14}$$

(the terms in (13) involving e_j and k_j cancel in the sum).

3 Lower bound for the elastic energy

In the continuum theory of nematic liquid crystals [12], the elastic, or Frank-Oseen, energy of a configuration $\mathbf{n}$ is given by

$$E(\mathbf{n}) = \int_P \big[K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{\mathbf{curl}}\mathbf{n})^2 + K_3(\mathbf{n}\times\operatorname{\mathbf{curl}}\mathbf{n})^2 \\ + K_4 \operatorname{div}\left((\mathbf{n}\cdot\nabla)\mathbf{n} - (\operatorname{div}\mathbf{n})\mathbf{n}\right)\big]\, dV. \tag{15}$$

Tangent boundary conditions imply that the contribution from the K_4-term, which is a pure divergence, vanishes. In the so-called one-constant approximation, the remaining elastic constants K_1, K_2 and K_3 are taken to be the same. In this case, (15) simplifies to

$$E(\mathbf{n}) = \int_P (\nabla\mathbf{n})^2\, dV = K\int_P \sum_{j=1}^{3} (\partial_j\mathbf{n})^2\, dV. \tag{16}$$

We shall use the one-constant approximation in what follows.

Let $E_{\min}(e, k, \Omega)$ denote the minimum (infimum) energy for configurations with reflection-symmetric topology (e, k, Ω). In [7] we obtained the lower bound

$$E_{\min}(e, k, \Omega) \geq 8L_z|\Omega|. \tag{17}$$

In view of (14), this may be written as

$$E_{\min}(e, k, \Omega) \geq 4\pi L_z \left| \sum_{\sigma} w_\sigma \right|. \tag{18}$$

Here we derive a new lower bound which, in general, is an improvement on (17).

Theorem 3.1.

$$E_{min}(e, k, \Omega) \geq 4\pi L_z \sum_{\sigma} |w_\sigma|. \tag{19}$$

Proof. Let $\mathbf{n}$ be a configuration with reflection-symmetric topology (e, k, Ω) for which the energy (16) is finite. As shown in [6], we can, without loss of generality, take $\mathbf{n}$ to be smooth (smooth configurations are dense in the space of finite-energy configurations with respect to the energy norm).

We can assume that the energy of $\mathbf{n}$ in R is not more than its energy in any other octant of the prism (we can replace $\mathbf{n}(\mathbf{r})$ by $\mathbf{n}(\mathcal{R} \cdot \mathbf{r})$ for a product $\mathcal{R}$ of reflections through mid planes; the reflected configurations have the same topology and energy as $\mathbf{n}$). Then

$$E(\mathbf{n}) \geq 8 \int_R |\nabla \mathbf{n}|^2 \, dV \geq 8 \int_{r \leq L_z/2} |\nabla \mathbf{n}|^2 \, dV, \tag{20}$$

where the last integral is taken over the positive octant of the ball of radius $L_z/2$ about the origin. Using the local inequality for the energy density [8, 6, 7],

$$(\nabla \mathbf{n})^2 \geq 2|\mathbf{D}| \geq 2|\mathbf{D} \cdot \hat{\mathbf{r}}|, \tag{21}$$

we get that

$$E(\mathbf{n}) \geq 16 \int_{r \leq L_z/2} |\mathbf{D}(\mathbf{r}) \cdot \hat{\mathbf{r}}| \, dV = 16 \int_0^{L_z/2} dr \int_{\mathbf{r} \in C_r} |\mathbf{D}(\mathbf{r}) \cdot \hat{\mathbf{r}}| \, dS_r. \tag{22}$$

Here, C_r is the positive octant of the sphere of radius r about the origin, with area element dS_r.

We partition C_r into preimages of the octants O_σ of S^2, writing

$$E(\mathbf{n}) \geq 16 \int_0^{L_z/2} dr \int_{\mathbf{r}\in C_r} \left(\sum_\sigma \int_{O_\sigma} \mathbf{ds}\, \delta_{S^2}(\mathbf{n}(\mathbf{r}), \mathbf{s}) \right) |\mathbf{D}(\mathbf{r}) \cdot \hat{\mathbf{r}}|\, dS_r. \tag{23}$$

Here δ_{S^2} is the normalised Dirac delta-function on S^2, so that $\int_{O_\sigma} \mathbf{ds}\, \delta_{S^2}(\mathbf{n}(\mathbf{r}), \mathbf{s})$ equals one if $\mathbf{n}(\mathbf{r}) \in O_\sigma$ and is zero otherwise. We interchange the integrals over $\mathbf{r} \in C_r$ and $\mathbf{s}$ and take the absolute value outside these integrals to obtain

$$E(\mathbf{n}) \geq 16 \int_0^{L_z/2} dr \sum_\sigma \left| \int_{O_\sigma} \mathbf{ds} \int_{\mathbf{r}\in C_r} \delta_{S^2}(\mathbf{n}(\mathbf{r}), \mathbf{s}) \mathbf{D}(\mathbf{r}) \cdot \hat{\mathbf{r}}\, dS_r \right|. \tag{24}$$

For $\mathbf{s}$ a regular value of $\mathbf{n}$ (by Sard's theorem, regular values are of full measure), we get that

$$\int_{\mathbf{r}\in C_r} \delta_{S^2}(\mathbf{n}(\mathbf{r}), \mathbf{s})\, dS_r = \sum_p |\det d\mathbf{n}_{C_r}(\mathbf{r}_p)|^{-1} = \sum_p |\mathbf{D}(\mathbf{r}_p) \cdot \hat{\mathbf{r}}|^{-1}, \tag{25}$$

where the sum is taken over the preimages $\mathbf{r}_p \in C_r$ of $\mathbf{s}$, and we have used (6). Substituting into (24), we get that

$$E(\mathbf{n}) \geq 16 \int_0^{L_z/2} dr \sum_\sigma \left| \int_{O_\sigma} \mathbf{ds} \sum_p \operatorname{sgn}(\mathbf{D}(\mathbf{r}_p) \cdot \hat{\mathbf{r}}) \right|. \tag{26}$$

From (11), the sum over p is just the wrapping number $w(\mathbf{s}) = w_\sigma$, so that the integral over $\mathbf{s}$ trivially gives a factor of $\pi/2$ (the area of O_σ). Then the integral over r trivially gives a factor of $L_z/2$. The required result (19) follows.

$\square$

4 Conformal and anticonformal topologies

The new bound (19) agrees with the previous bound (18) for topologies where $\sum_\sigma |w_\sigma| = |\sum_\sigma w_\sigma|$, ie where the nonzero wrapping numbers all have the same sign. We will say that a reflection-symmetric topology is *conformal* if $w_\sigma \leq 0$ for all σ, *anticonformal* if $w_\sigma \geq 0$ for all σ, and *nonconformal* if neither of these conditions holds. Thus, the new bound constitutes an improvement for nonconformal topologies.

It is useful to characterise the conformal and anticonformal topologies directly in terms of the invariants (e, k, Ω).

Proposition 4.1. *Define functions* $\Omega_\chi(e,k)$*, where* $\chi = \pm$*, as follows:*

For $\chi e_x e_y e_z = 1$*,*

$$\Omega_\chi(e,k) = 2\pi \sum_j |k_j| + 2\pi \begin{cases} +\frac{7}{4}, & \text{if } \chi e_j k_j \le 0 \text{ for all } j, \\ -\frac{1}{4}, & \text{otherwise.} \end{cases} \tag{27}$$

For $\chi e_x e_y e_z = -1$*,*

$$\Omega_\chi(e,k) = 2\pi \sum_j |k_j| - 2\pi \begin{cases} +\frac{7}{4}, & \text{if } \chi e_j k_j < 0 \text{ for all } j, \\ -\frac{1}{4}, & \text{otherwise.} \end{cases} \tag{28}$$

Then the reflection-symmetric topology (e,k,Ω) *is conformal if and only if* $\Omega \le -\Omega_-(e,k)$ *and anticonformal if and only if* $\Omega \ge \Omega_+(e,k)$*. If equality obtains, ie* $\Omega = -\Omega_-(e,k)$ *or* $\Omega = \Omega_+(e,k)$*, then at least one wrapping number must vanish.*

Proof. The condition $\chi w_\sigma \ge 0$ for all σ is equivalent to (e,k,Ω) being conformal ($\chi = -$) or anticonformal ($\chi = +$). From (13), $\chi w_\sigma \ge 0$ for all σ if and only if $\chi\Omega \ge \Omega_\chi(e,k)$, where

$$\Omega_\chi(e,k) = 2\pi \max_\sigma \left(-\chi \sum_j \sigma_j k_j + \chi e_x e_y e_z \times \begin{cases} +\frac{7}{4}, & \text{if } \sigma_j = e_j \text{ for all } j \\ -\frac{1}{4}, & \text{otherwise} \end{cases} \right), \tag{29}$$

with $\chi\Omega = \Omega_\chi(e,k)$ if and only if $w_\sigma = 0$ for some σ. In (29), to realise the maximum we may take, for all j such that $k_j \ne 0$, $\sigma_j = -\chi \operatorname{sgn} k_j$, and thereby replace $-\chi\sigma_j k_j$ by $|k_j|$ for all j. Thus,

$$\Omega_\chi(e,k) = 2\pi \sum_j |k_j| + \max_{\sigma_j \,|\, k_j = 0} \chi e_x e_y e_z \times \begin{cases} +\frac{7}{2}\pi, & \text{if } \sigma_j = e_j \text{ for all } j, \\ -\frac{1}{2}\pi, & \text{otherwise} \end{cases}. \tag{30}$$

It remains to maximise the second term in (30) with respect to the σ_j's for which $k_j = 0$. Suppose that $\chi e_x e_y e_z = 1$. Then, provided $\sigma_j = e_j$ for all $k_j \ne 0$, ie provided $-\chi \operatorname{sgn} k_j = e_j$ for all $k_j \ne 0$, the maximum value attained by the second term in (30) is $7\pi/2$. Otherwise, the maximum is $-\pi/2$. This is in accord with (27). Next, suppose that $\chi e_x e_y e_z = -1$. The maximum value attained by the second term in (30) is $\pi/2$ unless all the k_j's are nonzero and $-\chi \operatorname{sgn} k_j = e_j$, in which case the maximum is $-7\pi/2$. This is in accord with (28). □

In [7] we introduced certain reflection-symmetric configurations in P which we called conformal and anticonformal. We show next that the conformal and anticonformal topologies are precisely those which have conformal and anticonformal representatives. To proceed, we briefly recall the properties of conformal configurations ([6]) (as discussed below, the treatment of anticonformal configurations is analogous). A reflection-symmetric configuration $\mathbf{n}$ is said to be *conformal* if, in the prism octant R, i) $\mathbf{n}$ is radially constant, ie $\mathbf{n}(\lambda\mathbf{r}) = \mathbf{n}(\mathbf{r})$, and ii) $\mathbf{n}$ is conformal, ie the map $\mathbf{t} \mapsto \nabla_t\mathbf{n}(\mathbf{r})$ from vectors $\mathbf{t}$ orthogonal to $\hat{\mathbf{r}}$ to vectors $\nabla_t\mathbf{n}(\mathbf{r})$ orthogonal to $\mathbf{n}(\mathbf{r})$ preserves orientation, angles and ratios of lengths (or else vanishes).

Conformal configurations are conveniently represented via stereographic projection as analytic functions $f(w)$,

$$\left(\frac{n_x + in_y}{1 + n_z}\right)(x, y, z) = f\left(\frac{x + iy}{r + z}\right). \tag{31}$$

The domain of $f(w)$ is the quarter-unit-disk Q given by $|w| \leq 1$, $0 \leq \operatorname{Re} w \leq 1$ and $0 \leq \operatorname{Im} w \leq 1$. The boundary of Q consists of the real interval $0 \leq w \leq 1$ (which corresponds to the xz-face of R), the imaginary interval $0 \leq -iw \leq 1$ (which corresponds the yz-face), and the circular arc $|w| = 1$, where $0 \leq \arg w \leq \pi/2$ (which corresponds to the xy-face). Tangent boundary conditions imply that i) $f(w)$ is real for w real, ii) $f(w)$ is imaginary for w imaginary, and iii) $|f(w)| = 1$ if $|w| = 1$. Assuming that $f(w)$ has a meromorphic extension to the extended complex plane, these conditions imply that if w_* is a zero of f, then $-w_*$ and $\bar{w}_*$ are zeros, while $1/\bar{w}_*$ is a pole. The meromorphic functions which satisfy these conditions are rational functions of the following form:

$$f(w) = \epsilon w^n \prod_{j=1}^{a} \left(\frac{w^2 - r_j^2}{r_j^2 w^2 - 1}\right)^{\rho_j} \prod_{k=1}^{b} \left(\frac{w^2 + s_k^2}{s_k^2 w^2 + 1}\right)^{\sigma_k} \times$$
$$\times \prod_{l=1}^{c} \left(\frac{(w^2 - t_l^2)(w^2 - \bar{t}_l^2)}{(t_l^2 w^2 - 1)(\bar{t}_l^2 w^2 - 1)}\right)^{\tau_l}. \tag{32}$$

Here, $\epsilon = \pm 1$ and n, an odd integer, gives the order of the zero or pole of f at the origin. a is the number of zeros of f ($\rho_j = 1$) and poles of f ($\rho_j = -1$) on the real interval $(0, 1)$, with positions r_j ordered so that $0 < r_1 \leq \cdots \leq r_a < 1$. Similarly, b is the number of zeros of f ($\sigma_k = 1$) and poles of f ($\sigma_k = -1$) on the imaginary interval $(0, i)$, with positions is_k ordered so that $0 < s_1 \leq \cdots \leq s_b < 1$. Finally, c is the number of zeros of f ($\tau_l = 1$) and poles of f ($\tau_l = -1$) in the interior of Q, with positions t_l.

The edge signs, kink numbers and trapped area of conformal configurations are given by

$$e_x = \epsilon(-1)^a, \;\; e_y = \epsilon(-1)^b(-1)^{(n-1)/2}, \;\; e_z = \text{sgn } n, \tag{33}$$

$$\begin{aligned}
k_x &= -\tfrac{1}{2}(-1)^b e_y \left(\sum_{k=1}^{b} (-1)^k \sigma_k + \tfrac{1}{2}(1-(-1)^b)e_z \right), \\
k_y &= -\tfrac{1}{2}(-1)^a e_x \left(\sum_{j=1}^{a} (-1)^j \rho_j + \tfrac{1}{2}(1-(-1)^a)e_z \right), \\
k_z &= \tfrac{1}{4}\left(e_x e_y - n\right) - \tfrac{1}{2}\sum_{j=1}^{a}\rho_j - \tfrac{1}{2}\sum_{k=1}^{b}\sigma_k - \sum_{l=1}^{c}\tau_l,
\end{aligned} \tag{34}$$

and

$$\Omega = -\tfrac{1}{2}(|n| + 2(a+b) + 4c)\pi. \tag{35}$$

As explained in [7], the expressions for the edge signs and the trapped area are easily derived (in particular, (35) follows from consideration of the degree of f on the extended complex plane). A derivation of the expression for the kink numbers, which was deferred in [7], is given here in Appendix A.

Clearly, a conformal configuration has a conformal topology; the orientation-reversing property ensures that the wrapping numbers cannot be positive. Below we establish the converse fact; every conformal topology (e, k, Ω) has a conformal representative. The demonstration splits into four cases according to the sign of $e_x e_y e_z$ and of $e_j k_j$. In each case we exhibit the parameter values, expressed in terms of e, k and Ω, for a particular conformal configuration. It is then straightforward to verify – we omit the explicit demonstration – that the specified parameters are admissable (ie, that n is an odd integer; a, b, c are nonnegative integers; ϵ, ρ_j, σ_k, τ_l are signs), and that, with these parameters, the values of the invariants given by (33)– (35) are just (e, k, Ω). Deriving the exhibited values involves a systematic and slightly tedious investigation of (33)– (35). For the sake of brevity, these details are also omitted.

Case 1a. $e_x e_y e_z = 1$ *and* $e_j k_j > 0$ *for all* j. Let

$$\begin{gathered}
\epsilon = -e_x, \quad n = e_z, \\
a = 2|k_y| - 1, \quad \rho_j = (-1)^j e_z, \\
b = 2|k_x| - 1, \quad \sigma_k = (-1)^k e_z, \\
c = -\tfrac{1}{2\pi}\Omega - |k_x| - |k_y| + \tfrac{3}{4}, \quad \tau_l = \begin{cases} -e_z, & l < |k_z|, \\ (-1)^l, & l \geq |k_z|. \end{cases}
\end{gathered} \tag{36}$$

Note that (13) implies that $c-(|k_z|-1)$ is nonnegative and even. Here and in the cases to follow, we do not specify the positions of the zeros and poles explicitly.

Case 1b. $e_x e_y e_z = 1$ and $e_j k_j \leq 0$ for some j. Without loss of generality, we may assume that $j = z$. This follows from considering the fractional linear transformation

$$r(w) = \frac{i-w}{i+w} \tag{37}$$

which maps Q onto itself while cyclically permuting its vertices (r corresponds to the $2\pi/3$-rotation on S^2 about the axis (1,1,1)). Therefore, if f is a conformal configuration, so is $\tilde{f}$ given by

$$\tilde{f} = r \circ f \circ r^{-1}. \tag{38}$$

It is easily verified that $\tilde{f}$ and f have the same trapped areas while their edge signs and kink numbers are related by cyclic permutation,

$$\tilde{e} = (e_z, e_x, e_y), \quad \tilde{k} = (k_z, k_x, k_y). \tag{39}$$

Letting $e_z k_z \leq 0$, we take

$$\begin{gathered}
\epsilon = e_x, \quad n = (4|k_z|+1)e_z, \\
a = 2|k_y|, \quad \rho_j = -(-1)^j e_x \operatorname{sgn} k_y, \\
b = 2|k_x|, \quad \sigma_k = -(-1)^k e_y \operatorname{sgn} k_x, \\
c = -\tfrac{1}{2\pi}\Omega - |k_x| - |k_y| - |k_z| - \tfrac{1}{4}, \quad \tau_l = (-1)^l.
\end{gathered} \tag{40}$$

Note that (13) implies that c is nonnegative and even.

Case 2a. $e_x e_y e_z = -1$ and $e_j k_j < 0$ for some j. As in Case 1b, without loss of generality, we may take $e_z k_z < 0$. Let

$$\begin{gathered}
\epsilon = e_x, \quad n = -(4k_z + e_z), \\
a = 2|k_y|, \quad \rho_j = -(-1)^j e_x \operatorname{sgn} k_y, \\
b = 2|k_x|, \quad \sigma_k = -(-1)^k e_y \operatorname{sgn} k_x, \\
c = -\tfrac{1}{2\pi}\Omega - |k_x| - |k_y| - |k_z| + \tfrac{1}{4}, \quad \tau_l = (-1)^l.
\end{gathered} \tag{41}$$

Note that (13) implies that c is nonnegative and even.

Case 2b. $e_x e_y e_z = -1$ and $e_j k_j \geq 0$ for all j. Let

$$\begin{aligned} \epsilon &= e_x, \quad n = 3e_z, \\ a &= 2|k_y|, \quad \rho_j = e_z(-1)^j, \\ b &= 2|k_x|, \quad \sigma_k = e_z(-1)^k, \\ c = -\tfrac{1}{2\pi}\Omega - |k_x| - |k_y| - \tfrac{3}{4}, &\quad \tau_l = \begin{cases} -e_z, & l \leq |k_z| + 1, \\ (-1)^l, & l > |k_z| + 1. \end{cases} \end{aligned} \tag{42}$$

Note that (13) implies that $c - (|k_z| + 1)$ is nonnegative and even.

Anticonformal configurations are given by antianalytic functions, in analogy with the conformal case. Specifically, if $f(w)$ is a conformal configuration, then $\overline{f(w)}$ is anticonformal with invariants $(\bar{e}, \bar{k}, \bar{\Omega})$ given by

$$\bar{e} = (e_x, -e_y, e_z), \quad \bar{k} = (-k_x, k_y, -k_z), \quad \bar{\Omega} = -\Omega. \tag{43}$$

Thus, conformal and anticonformal configurations are in one-to-one correspondence. Also, given any (e, k, Ω) and $(\bar{e}, \bar{k}, \bar{\Omega})$ related as in (43), one can verify from (27) and (28) that $\Omega_+(\bar{e}, \bar{k}) = \Omega_-(e, k)$, so that $\bar{\Omega} \geq \Omega_+(\bar{e}, \bar{k})$ if and only if $\Omega \leq -\Omega_-(e, k)$. Thus, conformal and anticonformal topologies are in one-to-one correspondence, and representatives of every anticonformal topology may be obtained from complex conjugation of the associated conformal representative.

The preceding discussion may be summarised as follows:

Proposition 4.2. *A reflection-symmetric topology is conformal if and only if it contains a conformal configuration, and anticonformal if and only if it contains a anticonformal configuration.*

5 Upper bound for elastic energy

In [7] we showed that for a conformal or anticonformal topology (e, k, Ω),

$$E_{\min}(e, k, \Omega) \leq 8L|\Omega|. \tag{44}$$

where

$$L = (L_x^2 + L_y^2 + L_z^2)^{1/2}. \tag{45}$$

We note that the upper bound differs from the lower bound (17) by a factor, L/L_z, which depends only on the aspect ratios of the prism, and not on (e, k, Ω).

Here we derive an analogous upper bound for nonconformal topologies. To this end, we construct representatives $\mathbf{n}$. As in the conformal and anticonformal cases, we take these to be reflection-symmetric and radially constant in R. In R, $\mathbf{n}$ is taken to be of the form

$$\left(\frac{n_x + in_y}{1 + n_z}\right)(\mathbf{r}) = F(w, \bar{w}), \text{ where } w = \frac{x + iy}{r + z}. \tag{46}$$

We take F to be a juxtaposition of analytic and antianalytic domains (in which the local estimate (21) for the energy density becomes an equality), separated by an interpolating domain of small energy. For definiteness, we take $\Omega < 0$ (the case $\Omega > 0$ is treated analogously). Let f denote the conformal configuration with topology $(e, k, -\Omega_-(e, k))$, so that f is the conformal configuration with the largest trapped area compatible with e and k. Let w_0 denote a point in the interior of Q, and let $D_\epsilon(w_0) = \{w \,|\, |w - w_0| < \epsilon\}$ denote the open ϵ-disk about w_0. Choose w_0 and ϵ so that $D_{2\epsilon}(w_0)$ is contained in Q and contains no poles of f. Let

$$W = \tfrac{1}{4\pi}(\Omega + \Omega_-(e, k)). \tag{47}$$

Since (e, k, Ω) is nonconformal, W is a positive integer. We let

$$F(w, \bar{w}) = \begin{cases} f(w), & w \in Q - D_{2\epsilon}(w_0), \\ sf(w) + (1 - s)(f(w_0) + (w - w_0)^W), & w \in D_{2\epsilon}(w_0) - D_\epsilon(w_0), \\ f(w_0) + \epsilon^{2W}(\bar{w} - \bar{w}_0)^{-W}, & w \in D_\epsilon(w_0), \end{cases} \tag{48}$$

where

$$s(w, \bar{w}) = \frac{|w - w_0| - \epsilon}{\epsilon} \tag{49}$$

(so that s varies between 0 and 1 as $|w - w_0|$ varies between ϵ and 2ϵ). Thus, in $Q - D_{2\epsilon}(w_0)$, F coincides with f and therefore is conformal, while in $D_\epsilon(w_0)$ it is anticonformal.

Let us verify that F has the required topology. Since it coincides with f on the boundary of Q, F has the same edge signs and kink numbers as f, namely e and k. As for the trapped area, from (4) and (46) it is straightforward to derive the general expression

$$\Omega(F) = \int_Q 4\frac{|\partial_{\bar{w}} F|^2 - |\partial_w F|^2}{(1 + |F|^2)^2}\, d^2w. \tag{50}$$

(50) can be evaluated by dividing the domain of integration as in (48). The contribution from $Q - D_{2\epsilon}(w_0)$ is, to $O(\epsilon^2)$, just the trapped area of f, namely

$-\Omega_-(e,k)$ (substituting f for F in (50), the contribution from $D_{2\epsilon}(w_0)$ is $O(\epsilon^2)$). Consider next the contribution from the disk $D_\epsilon(w_0)$. Here $F = f(w_0) + \epsilon^{2W}(\bar{w} - \bar{w}_0)^{-W}$, so that F covers the extended complex plane, apart from an ϵ^W-disk about $f(w_0)$, W times with positive orientation. It follows that the contribution to (50) is, to within $O(\epsilon^W)$ corrections, $4\pi W$. The remaining contribution, from the annulus $D_{2\epsilon}(w_0) - D_\epsilon(w_0)$, is $O(\epsilon^2)$. This is because the area of the annulus is $O(\epsilon^2)$, while the integrand in (50) may be bounded independently of ϵ (by assumption, f has no poles in $D_{2\epsilon}(w_0)$). Since the trapped area is an odd multiple of $\pi/2$, it follows that, for small enough ϵ,

$$\Omega(F) = -\Omega_-(e,k) + 4\pi W = \Omega. \tag{51}$$

By estimating the energy of the nonconformal representatives we can obtain the following upper bound for $E_{\min}(e,k,\Omega)$:

Theorem 5.1. *Let (e,k,Ω) denote a nonconformal topology. Then*

$$E_{min}(e,k,\Omega) \le 36\pi L \sum_\sigma |w_\sigma|. \tag{52}$$

Proof. From (16) and (46) one can derive the general expression for the energy,

$$E(F) = 16 \int_Q 4|\mathbf{r}(w)| \frac{|\partial_{\bar{w}} F|^2 + |\partial_w F|^2}{(1+|F|^2)^2}\, d^2 w, \tag{53}$$

where $\mathbf{r}(w)$ is the point on the boundary of R which has w as its stereographic projection. Since $|\mathbf{r}(w)| \le L/2$, it follows that

$$E(F) \le 8L\mathcal{A}(F), \tag{54}$$

where

$$\mathcal{A}(F) = \int_Q 4 \frac{|\partial_{\bar{w}} F|^2 + |\partial_w F|^2}{(1+|F|^2)^2}\, d^2 w. \tag{55}$$

$\mathcal{A}(F)$ represents the unoriented area of $\mathbf{n}(C_r)$. The expression (55) for $\mathcal{A}(F)$ differs from the expression (50) for $\Omega(F)$ in the relative sign of the w- and $\bar{w}$-derivative terms. (Thus, for conformal and anticonformal configurations, one obtains the estimate (44).) Arguing as for (51), we have that

$$\mathcal{A}(F) \le |\Omega_-(e,k)| + 4\pi W. \tag{56}$$

From (14), this may be written as

$$\mathcal{A}(F) \le 4\pi W - \tfrac{1}{2}\pi \sum_\sigma w_{\sigma -}, \tag{57}$$

where $w_{\sigma -}$ are the (nonpositive) wrapping numbers of f. From (13) and (47), the $w_{\sigma -}$'s are related to the wrapping numbers of F, denoted w_σ, according to

$$w_{\sigma -} = w_\sigma - W. \tag{58}$$

Substituting into (57), we get that

$$\mathcal{A}(F) \leq 4\pi W + \tfrac{1}{2}\pi \sum_\sigma (W - w_\sigma) \leq 8\pi W + \tfrac{1}{2}\pi \sum_\sigma |w_\sigma|. \tag{59}$$

One easily establishes the estimate

$$2W \leq \sum_\sigma |w_\sigma|. \tag{60}$$

Indeed, since $\Omega < 0$ by assumption, it follows from (14) that

$$\sum_\sigma w_\sigma < 0. \tag{61}$$

Since f has trapped area $-\Omega_-(e,k)$, it follows from Proposition 4.1 that there is at least one octant, say σ_0, in which f has zero wrapping number. From (58), $w_{\sigma_0} = W$. Let $\sum_\sigma'$ denote the sum over octants with σ_0 omitted. Then

$$\sum_\sigma{}' w_\sigma < -W. \tag{62}$$

It follows that

$$\sum_\sigma |w_\sigma| = \sum_\sigma{}' |w_\sigma| + W \geq \left| \sum_\sigma{}' w_\sigma \right| + W \geq 2W. \tag{63}$$

Substituting (63) into (57), we get that

$$\mathcal{A}(F) \leq 9 \times \tfrac{1}{2}\pi \sum_\sigma |w_\sigma|. \tag{64}$$

The required result, (52), follows from substitution into (54). □

6 Discussion

For nonconformal topologies, the ratio of the upper and lower bounds for $E_{\min}$, as given by (52) and (19), is $9L/L_z$. By finding representatives of

lower energy, it might be possible to obtain a ratio closer to the conformal/anticonformal result, L/L_z (which can be further improved by more accurate estimates of the energy of the representatives [7]).

In [6], we described, for conformal and anticonformal topologies, a transition in topologically nontrivial equilibrium (infimum-energy) configurations, from singular, in the case of a cubic domain, to smooth, as the prism aspect ratios are varied. Singular configurations, when they appear, are limits of configurations which differ from the topologically simplest "unwrapped" configurations in thin tubes along the prism edges. It would be interesting to investigate whether similar transitions occur for nonconformal topologies. The nonconformal representatives differ from conformal/anticonformal configurations only in a tube (a disk in the two-dimensional stereographic description (48)), and depending on the aspect ratios, it may be energetically advantageous for these tubes to collapse to edge singularities, or not.

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A Kink numbers of conformal configurations

Taking $\mathbf{n}$ to be a conformal configuration with stereographic projection f given by (32), we derive formulas for the kink numbers $k = (k_x, k_y, k_z)$ in terms of the parameters of f.

Formulas for k_x and k_y. For definiteness, consider the calculation of k_y. Let $\mathbf{r}(\tau)$, $0 \le \tau \le 1$, denote a small quarter-circular arc on the xz-face of R starting on the z-axis and ending on the x-axis (so that $\mathbf{r}(\tau)$ is positively oriented with respect to the outward normal $-\hat{\mathbf{y}}$ through the centre of the face). Let $\boldsymbol{\nu}(\tau) = \mathbf{n}(\mathbf{r}(\tau))$. Then $\boldsymbol{\nu}(\tau)$ describes a curve on S^2 along the great circle in the xz-plane, starting from $e_z\hat{\mathbf{z}}$ and ending at $e_x\hat{\mathbf{x}}$. k_y is the winding number of $\boldsymbol{\nu}(\tau)$ relative to the shortest arc joining $e_z\hat{\mathbf{z}}$ to $e_x\hat{\mathbf{x}}$, with anticlockwise windings about $-\hat{\mathbf{y}}$ taken as positive. k_y is given by the number of times $\boldsymbol{\nu}(\tau)$ crosses a given point, say $\hat{\mathbf{z}}$, counted with a sign according to orientation. Let τ_p denote the parameter values at these crossings. Assuming that $\boldsymbol{\nu}'(\tau_p) \ne 0$, we get that

$$k_y = -\sum_{\tau_p > 0} \operatorname{sgn}(\boldsymbol{\nu}'(\tau_p)\cdot\hat{\mathbf{x}}) + \tfrac{1}{2}(1+e_z)\cdot\tfrac{1}{2}(e_x - \operatorname{sgn}(\boldsymbol{\nu}'(0)\cdot\hat{\mathbf{x}})). \qquad (65)$$

If $e_z = 1$ then $\boldsymbol{\nu}(0) = \hat{\mathbf{z}}$; the last term in (65) accounts for a possible contri-

bution in this case. There is no contribution if $\operatorname{sgn}(\boldsymbol{\nu}'(0)\cdot\hat{\mathbf{x}}) = e_x$, as for the shortest arc joining $\hat{\mathbf{z}}$ to $e_x\hat{\mathbf{x}}$ (for which $k_y = 0$). Otherwise, the initial point constitutes a crossing with sign e_x.

Under stereographic projection, $\mathbf{r}(\tau)$ corresponds to $w(\tau) = \tau$, the crossing $\boldsymbol{\nu}(\tau_p) = \hat{\mathbf{z}}$ corresponds to $f(\tau_p) = 0$, and $\operatorname{sgn}(\boldsymbol{\nu}'(\tau_p)\cdot\hat{\mathbf{x}})$ corresponds to $\operatorname{sgn} f'(\tau_p)$. The zeros of f on the real interval $(0,1)$ are given by the r_j's with $\rho_j = 1$. Thus, (65) becomes

$$k_y = -\sum_{j\,|\,\rho_j=1} \operatorname{sgn} f'(r_j) + \tfrac{1}{2}(1+e_z)\cdot\tfrac{1}{2}(e_x - \operatorname{sgn} f'(0)). \tag{66}$$

For simplicity, let us assume that the r_j's are all distinct and ordered so that $0 < r_1 < \cdots < r_a < 1$. In this case, for $\rho_j = 1$, $f'(r_j) \neq 0$, and from (32), we have that

$$\operatorname{sgn} f'(r_j) = \operatorname{sgn}\left[\epsilon\frac{2r_j}{r_j^4 - 1}\prod_{\substack{m=1\\ m\neq j}}^{a}\left(\frac{r_j^2 - r_m^2}{r_m^2 r_j^2 - 1}\right)^{\rho_m}\right] = \epsilon(-1)^j. \tag{67}$$

If $e_z = 1$, n is positive, and $w = 0$ is also a zero of f. As $f'(0)$ vanishes if $n > 1$, we replace $\operatorname{sgn} f'(0)$ by $\lim_{w\to 0}\operatorname{sgn} f(w) = \epsilon$. (66) becomes

$$k_y = -\epsilon\sum_{j=1}^{a}(-1)^j\cdot\tfrac{1}{2}(1+\rho_j) + \tfrac{1}{2}(1+e_z)\cdot\tfrac{1}{2}(e_x - \epsilon) \tag{68}$$

Recalling that $e_x = \epsilon(-1)^a$, with some further straightforward manipulation we obtain

$$k_y = -\tfrac{1}{2}(-1)^a e_x\left(\sum_{j=1}^{a}(-1)^j\rho_j + \tfrac{1}{2}e_z(1-(-1)^a)\right), \tag{69}$$

which is just the expression given in (34). In fact, (69) holds even if some of the r_j's coincide.

The expression for k_x is similarly derived, with $\mathbf{r}(\tau)$ taken to be a quarter-circular arc on the zy-face of R with projection $w = i(1-\tau)$. Details are omitted.

Formula for k_z. Let $\mathbf{r}(\tau)$, $0 \le \tau \le 1$, denote a small quarter-circular arc on the xy-face of R starting on the x-axis and ending on the y-axis (so that $\mathbf{r}(\tau)$ is positively oriented with respect to the outward normal $-\hat{\mathbf{z}}$ through the centre of the face). Under stereographic projection, $\mathbf{r}(\tau)$ corresponds

to $w(\tau) = \exp(i\pi\tau/2)$, and $\mathbf{n}(\mathbf{r}(\tau))$ to $f(\exp(i\pi\tau/2))$. k_z is the winding number of $f(\exp(i\pi\tau/2))$ on the unit circle in the complex plane relative to the shortest arc joining $e_x\hat{\mathbf{x}}$ to $e_y\hat{\mathbf{y}}$. Clockwise windings are taken as positive. It follows that

$$k_z = -\tfrac{1}{2\pi} \left(\arg f(\exp(i\pi/2)) - \arg f(0)\right) + \tfrac{1}{4} \operatorname{sgn}(e_x e_y), \tag{70}$$

where $\arg f(\exp(i\pi\tau/2))$ is taken to be continuous in τ and the last term ensures the winding number is zero for the shortest arc joining $e_x\hat{\mathbf{x}}$ to $e_y\hat{\mathbf{y}}$. Referring to (32), each factor of the form $[(w^2 \pm p^2)/(p^2w^2 \pm 1)]^\xi$ contributes $\xi\pi$ to the change in $\arg f$ in (70), while z^n contributes $n\pi/2$. Thus we get

$$k_z = -\tfrac{1}{2}\sum_{j=1}^{a} \rho_j - \tfrac{1}{2}\sum_{k=1}^{b} \sigma_k - \sum_{l=1}^{c} \tau_l - \tfrac{1}{4}(n - e_x e_y), \tag{71}$$

as in (34).

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